Dynamical Transition from Triplets to Spinon Excitations: A Series Expansion Study of the $J_1 - J_2 - \delta$ spin-half chain

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Abstract

We study the spin-half Heisenberg chain with alternating nearest neighbor interactions $J_1(1+\delta)$ and $J_1(1-\delta)$ and a uniform second neighbor interaction $J_2 = y(1-\delta)$ by series expansions around the limit of decoupled dimers ($\delta = 1$). By extrapolating to $\delta = 0$ and tuning y, we study the critical point separating the power-law and spontaneously dimerized phases of the spin-half antiferromagnet. We then focus on the disorder line $y = 0.5$, $0 \leq \delta \leq 1$, where the ground states are known exactly. We calculate the triplet excitation spectrum, their spectral weights and wavevector dependent static susceptibility along this line. It is well known that as $\delta \to 0$, the spin-gap is still non-zero but the triplets are replaced by spinons as the elementary excitations. We study this dynamical transition by analyzing the series for the spectral weight and the static susceptibility. In particular, we show that the spectral weight for the triplets vanishes and the static spin-susceptibility changes from a simple pole at imaginary wavevectors to a branch cut at the transition.

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I. INTRODUCTION

The study of quantum-disordered ground states of low dimensional spin systems, with an absence of long-range magnetic order and a gap to spin excitations, has attracted considerable interest recently [1]. A question of fundamental importance in the field is the nature of elementary excitations in these phases. These spin excitations could be related to simple spin-flips, in which case they should carry spin-one, or they could represent free spin-half excitations in an otherwise spinless background. The existence of such spin-half excitations or spinons, in $d > 1$ lattice models remains an outstanding open question [2,3]. Thus it is important to develop suitable numerical schemes that can look for such spin-half excitations. The purpose of this paper is to test such a series expansion based method on a 1-dimensional model, where the existence of such excitations is well known, and to study the properties of the transition.

The $J_1 - J_2 - \delta$ spin-half chain is given by the Hamiltonian:

$$\mathcal{H} = J_1 \sum_i (1 + (-1)^i \delta) \vec{S}_i \cdot \vec{S}_{i+1} + J_2 \sum_i \vec{S}_i \vec{S}_{i+2} \tag{1}$$

This model has been a subject of many theoretical studies [4–6]. In particular for $\delta = 0$, it is well known that the model undergoes a phase transition from a critical phase at small J_2/J_1 to a spontaneously dimerized phase at large J_2/J_1. The critical value of J_2/J_1 has been accurately computed to be $(J_2/J_1)_c = 0.2411$ [7]. It is also well known that for the nearest neighbor spin-half chain, the presence of marginal operators lead to logarithmic corrections to various correlation functions [8]. It has been argued that these marginal operators are absent at the transition to the dimerized phase [9] and in this case the logarithmic corrections should also go away. This result has been confirmed in previous numerical studies [10]. Here, we present results from series analysis, which lend further support to it.

The primary focus of this paper is on the excitation spectra along a special line in the parameter space, where the ground state is known exactly. Along this line $0 \leq 2J_2/J_1 = 1 - \delta < 1$, this model has a unique ground state consisting of singlet pairs between spins at S_{2i} and S_{2i+1} [5]. Having the simple ground states with no quantum fluctuations allows us to focus on the elementary excitations of the system. In the disconnected dimer limit, $J_2 = J_1(1-\delta)/2 = 0$, the elementary excitations are localized triplets, where one of the spin-pair (S_{2i}, S_{2i+1}) is excited to a triplet. These triplet excitations develop a dispersion for $\delta \neq 1$, but remain well defined for all $\delta > 0$. At $\delta = 0$, the Hamiltonian has full translational symmetry, and from the well known results of Majumdar and Ghosh [4], this symmetry is spontaneously broken leading to two degenerate ground states. One of these two ground states is the same as the ground state for $\delta > 0$. In this case, the elementary excitations are spinons or domain walls with spin-half, which interpolate between the two ground states. This result was first established through the variational calculations of Shastry and Sutherland [5] and has since been confirmed by many authors [6].

A popular way to study the spinons to triplet transition occuring at small δ, is through the binding of spinon pairs due to the confining linear potential [11]. Here we will consider the opposite point of view and study the break up of the triplets into spinon pairs as δ goes to zero. Thus, this method allows one to look for spinon excitations, in models where there existence is not yet established, starting from a limit where only triplet excitations

exist. Recently such a search for spinons was carried out in the bilayer triangular-lattice Heisenberg model, where they were not found to be present [12].

Here we calculate the dispersion for the triplet excitations, their spectral weights and the wavevector dependent static susceptibility by series expansions around the disconnected dimer limit. The series analysis clearly confirms that as $\delta \to 0$, the spectral weights for the triplets vanishes (except very near the dispersion maximum at $k = \pi/2$, where in the spinon picture triplet bound states are known to exist). Furthermore, for $\delta \neq 0$, the static susceptibility has a simple pole at imaginary wavevectors, reflecting the quasiparticle nature of the triplet excitations. As $\delta \to 0$, this turns into a branch cut reflecting the absence of triplet quasiparticles. This study shows that the series expansion method is well suited to studying this transition. Since this method can easily be applied in higher dimensional systems, it gives us hope that it can be used to search for such spin-half excitations in those cases as well.

II. SERIES CALCULATIONS

To construct a series expansion around the limit of disconnected dimers in powers of

$$\lambda = \frac{1-\delta}{1+\delta},$$

one can rewrite the Hamiltonian in Eq. (1) in the following form:

$$\mathcal{H}/(1+\delta)J_1 = H_0 + \lambda V, \tag{2}$$

where the unperturbed Hamiltonian H_0 and the perturbation V are

$$H_0 = \sum_i \vec{S}_{2i} \cdot \vec{S}_{2i+1}, \tag{3}$$

$$V = \sum_i \vec{S}_{2i-1} \cdot \vec{S}_{2i} + y \sum_i \vec{S}_i \cdot \vec{S}_{i+2}. \tag{4}$$

y is related to J_2 by the relation

$$y = J_2/(1-\delta)J_1. \tag{5}$$

The expansions are developed for fixed values of y. The expansion methods for the wavevector dependent susceptibility [13,14], the triplet dispersion [15], and the spectral weight [16] are discussed in the literature. We will concentrate on the expansions for the following three different values of y:

(1) y =0, that is, without the second neighbor interaction;

(2) $y = y_c \equiv (J_2/J_1)_c = 0.2411$, that is, the system is at the critical point between gapped and gapless phases when $\lambda = 1$;

(3) $y = 0.5$, that is, the expansion is along the disorder line where the ground states are known exactly.

For the cases of $y = 0$ and 0.2411, the series have been computed to order λ^{23} for the ground state energy E_0, to order λ^{13} for antiferromagnetic susceptibility χ, and to order

λ^{11} for the triplet dispersion. There are only 12 graphs that contribute to the ground state energy and dispersion, and 14 graphs that contribute to the antiferromagnetic susceptibility. This considerably extends previous series expansions for this model [17,18].

For the case of $y = 0.5$, the series are carried out to order λ^{23} for the dispersion and to order λ^{17} for the susceptibility and the spectral weight. Due to some special symmetries of the model along the disorder line, a graph with n dimers contributes first in order $2(n-1)$. Thus only 8 graphs are needed to carry out the expansions complete to order λ^{17} and only 12 graphs to carry them out to order λ^{23}. For this model, the dispersion is symmetric around $q = \pi/2$, whereas the spectral weight at q, $W(q)$, is related to that at $\pi - q$ by the relation:

$$W(q)(1 - \cos(\pi - q)) = W(\pi - q)(1 - \cos q). \tag{6}$$

It is known that at $q = \pi/2$ the triplet dispersion and its spectral weight do not change with λ [6]. In the perturbation expansion this result is reflected in the fact that the expansion coefficients after the zeroeth order vanish. This serves as a further check on the calculations. The expansion coefficients would be available on request.

III. THE LOG CORRECTIONS IN THE POWER-LAW CORRELATED PHASE

For the case of $y < y_c$, the asymptotic behavior for ground state energy E_0, the energy gap Δ and antiferromagnetic susceptibility χ as $\delta \to 0$ ($\lambda \to 1$) are known to be [8]:

$$\begin{aligned} E_0(\delta) - E_0(\delta = 0) &\propto \frac{\delta^{4/3}}{|\ln \delta/\delta_0|^a} \\ \Delta(\delta) &\propto \frac{\delta^{2/3}}{|\ln \delta/\delta_0|^b} \\ \chi(\delta) &\propto \delta^{-2/3} |\ln \delta/\delta_0|^c \end{aligned} \tag{7}$$

with $a = 1$ and $b = 1/2$ [8], c has not been computed previously, as far as we are aware. Here, the logarithmic corrections are due to the marginal operators present in the model. It has been argued that these marginal operators are absent at the transition $y = y_c$ to the dimerized phase and we expect to have pure power-law asymptotic behavior there.

To study their behavior, the series were analysed using the standard Dlog Padé approximants. These approximants completely miss possible logarithmic corrections and thus can only lead to "effective" power-law exponents. The estimates for the critical points and exponents from the $[n/m]$ Dlog Padé approximants to the series for energy gap and antiferromagnetic susceptibility are given in Table I. From this table, we see that the critical point lies at $\lambda_c = 1.00(1)$ as expected. The "effective" critical exponents based on unbiased estimates (UB) and estimates with critical point biassed at $\lambda_c = 1$ (B) are given in Table II. We can see that for the case of $y = y_c$, the exponents agree with $\nu = \gamma = 2/3$ very well, This provides support to the argument that logarithmic corrections are absent here. For $y = 0$, the "effective" critical exponents for both Δ and χ are quite different from 2/3. As argued by Affleck and Bonner [19], the logarithmic corrections lead to "effective" exponents which vary slowly with the size of the system, or the length of the series. The estimated exponent values are in between the true values and the effective exponents for size 20 calculated by

them. One could also attempt to directly study the logarithmic singularity by multiplying the series by an appropriate power of $|\log \delta/\delta_0|$ before carrying out the Dlog Padé analysis. However, such an analysis will depend on the choice of δ_0. Such an analysis, varying δ_0 will not be attempted here. We note simply that choosing $\delta_0 = 1$, moves the effective exponents too far in the opposite direction.

IV. DISPERSION AND SPECTRAL WEIGHT ALONG THE DISORDER LINE

In this section, we begin by calculating the triplet dispersion as a function of δ. The dispersion-relations are shown for a number of δ values in figure 1. As one approaches $\delta = 0$, the gap in the spectrum stays robust: it approaches a constant with correction proportional to $(1-\lambda)^{2/3}$ [20], so in series extrapolation we transform the series to a new variable

$$\lambda' = 1 - (1-\lambda)^{2/3} \ , \tag{8}$$

to remove the singularity at $\lambda = 1$. For $\delta = 0$, the spectrum compares well with the lowest lying triplet-states in the variational calculation of Sutherland and Shastry [5]. As remarked earlier, at $q = \pi/2$ the triplet state remains unchanged as a function of δ.

The spectral weight of the triplets undergoes dramatic changes as the dynamical phase transition is approached. [20] Over substantial portions of the Brillouin zone, the spectral weight vanishes as $\delta \to 0$. A simple Dlog Padé analysis of the spectral weight series gives a vanishing spectral weight at λ slightly less than unity (δ slightly larger than zero), with an exponent which varies with the estimated critical point. It is difficult to determine this exponent accurately in an unbiassed manner. Since it is known that the spectral weights vanish as $\delta^{1/3}$ we adopt the following series extrapolation scheme: For a given wavevector, we generate the series in λ for the spectral-weight divided by $(1-\lambda)^{1/3}$. For a range of wavevectors the Padé approximant for the resulting series converges very well. For wavevectors close to $\pi/2$, the resulting series diverges as $\lambda \to 1$. This shows that for these q-values the spectral weight remains finite and is thus analyzed by a direct analysis of the spectral weight series [without the division by $(1-\lambda)^{1/3}$]. The resulting spectral weight at a few values of δ are shown in figure 2.

The susceptibility remains finite as $\delta \to 0$. Rather than look for a weak singularity in the susceptibility as $\delta \to 0$, we analyze the singular structure of the susceptibility at imaginary wavevectors. We expect that for $\delta \neq 0$, the susceptibility for small $k = \pi - q$ should have the form,

$$\chi(k) \approx \frac{A}{1 + k^2\xi^2} \tag{9}$$

So that at imaginary wavevector $k = i/\xi$, the susceptibility has a simple pole. However, as $\delta \to 0$, the spectrum now consists of two-spinon continuum, and the static susceptibility should now have a branch cut of the form [3],

$$\chi(k) \approx \frac{A}{(1 + k^2\xi^2)^{\alpha}}, \tag{10}$$

with an exponent $\alpha < 1$. Since the correlation length varies smoothly as a function of λ, this implies that if we consider the series for the susceptibility at a fixed imaginary wavevector,

κ, it should have a singularity at the λ value where the correlation length becomes i/κ. This singularity should be a simple pole (exponent unity) which should reduce to a branch cut (exponent less than unity) as $\lambda \to 1$ ($\delta \to 0$). We calculated the series for the susceptibility at a number of imaginary wavevectors κ, which were then analyzed by Padé approximants. The location of the singularity tells us the δ value at which the correlation length ξ equals i/κ. Thus this analysis gives both the correlation length and the exponent α as a function of our parameter δ. The resulting exponents and correlation length are plotted as a function of δ in Figure 3. The change in the nature of the singularity is clearly evident from the plot.

V. CONCLUSIONS

In this paper we have used series expansion methods to study the spin-half Heisenberg chain with bond alternation and nearest and second neighbor interactions. Our results are consistent with previous ones which show that "effective" exponents are modified due to logarithmic corrections in the power-law correlated phase of this model, but these modifications go away when the system is tuned to the critical point separating the power-law and spontaneously dimerized phases. We have also studied in detail the triplet spectra along the disorder line, where the ground states are known exactly. Our results provide clear evidence for a dynamical transition from triplet elementary excitations to spinons. The vanishing of the spectral weight and the change in the singularity structure of the wavevector dependent static susceptibility exhibit such a transition, while the ground state (and hence all equal-time correlation functions) remains free of singularities. This method should prove useful in looking for spin-half excitations in spin systems for $d > 1$.

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FIGURES

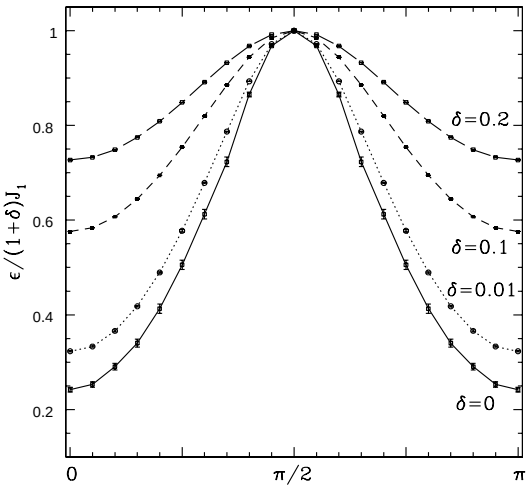

FIG. 1. The excitation spectrum $\epsilon(q)/(1+\delta)J_1$ for the $J_1 - J_2 - \delta$ spin-half chain along the disorder line, for $\delta = 0, 0.01, 0.1, 0.2$.

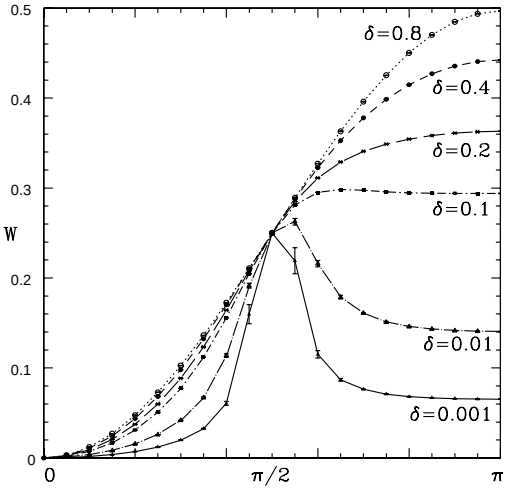

FIG. 2. The spetral weight $W(q)$ for the $J_1 - J_2 - \delta$ spin-half chain along the disorder line for $\delta = 0.001, 0.01, 0.1, 0.2, 0.4, 0.8$.

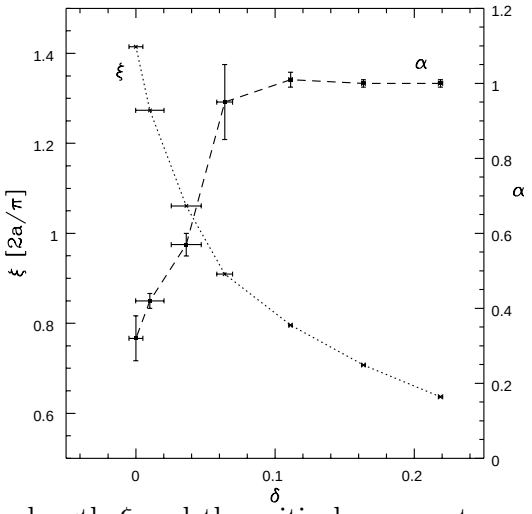

FIG. 3. The correlation length ξ and the critical exponent α, representing the singularity in the static susceptibility at imaginary wavevectors (Eq. 10) as a function of δ. Note that $\alpha = 1$ represents a simple pole and implies that the elementary excitations are triplets, whereas a smaller α represents a branch cut, and implies that the triplets have become composite objects.

TABLES

TABLE I. $[n/m]$ Dlog Padé approximants to the series for energy gap Δ and antiferromagnetic susceptibility χ. An asterisk denotes a defective approximant.

n	$[(n-2)/n]$ pole(residue)	$[(n-1)/n]$ pole(residue)	$[n/n]$ pole(residue)	$[(n+1)/n]$ pole(residue)	$[(n+2)/n]$ pole(residue)
			χ for $y=0$		
n= 2		0.9759(−0.749)	1.1109(−0.218)*	1.0143(−0.864)	0.9950(−0.771)
n= 3	0.9912(−0.786)	1.0079(−0.836)	1.0045(−0.822)	1.0033(−0.816)	1.0030(−0.814)
n= 4	1.0051(−0.825)	1.0029(−0.814)	1.0029(−0.813)	1.0040(−0.818)*	0.9973(−0.725)*
n= 5	1.0029(−0.813)	1.0029(−0.814)*	0.9905(−0.532)*	1.0021(−0.808)0	1.0012(−0.798)
n= 6	0.9982(−0.746)*	1.0012(−0.798)	1.0010(−0.797)		
			Δ for $y=0$		
n= 2		1.1088(0.970)	0.8216(0.322)	0.8374(0.348)	1.0986(1.243)
n= 3	0.9531(0.621)	0.9906(0.711)	1.0158(0.793)	0.9982(0.724)	1.0022(0.742)
n= 4	1.0495(0.986)	1.0047(0.751)	1.0016(0.738)	1.0018(0.740)	0.9896(0.501)*
n= 5	1.0021(0.741)	1.0018(0.739)	1.0017(0.739)		
			χ for $y=0.2411$		
n= 3	0.9931(−0.653)	1.0075(−0.712)	1.0002(−0.676)	1.0006(−0.678)	1.0005(−0.677)
n= 4	1.0004(−0.677)	1.0005(−0.677)	1.0005(−0.677)	1.0008(−0.678)*	1.0002(−0.674)
n= 5	1.0008(−0.680)	1.0005(−0.677)	1.0002(−0.674)	1.0001(−0.673)	1.0001(−0.673)
n= 6	1.0005(−0.677)	1.0001(−0.673)	1.0001(−0.673)		
			Δ for $y=0.2411$		
n= 2		1.6581(3.412)	1.4233(2.031)	0.6121(0.043)	0.7576(0.143)
n= 3	1.0588(0.737)	0.7751(0.190)*	1.1039(1.021)	0.9923(0.620)	1.0011(0.653)
n= 4	0.9562(0.531)	1.0082(0.680)	1.0002(0.649)	0.9960(0.632)	0.9945(0.626)
n= 5	1.0017(0.656)	1.0512(0.670)*	0.9944(0.626)*		

TABLE II. Estimates of "effective" critical exponents obtained by Dlog Padé approximants to the series for susceptibility χ, the energy gap Δ, and the difference of the ground state energy $E_0(\lambda) - E_0(\lambda = 1)$. Both unbiased estimates (UB) and estimates biased critical point $\lambda_c = 1$ (B) are listed.

series	$y=0$		$y=0.2411$	
	UB	B	UB	B
Δ	$\nu = 0.74(3)$	$\nu = 0.72(3)$	$\nu = 0.65(3)$	$\nu = 0.65(2)$
χ	$\gamma = 0.80(3)$	$\gamma = 0.78(2)$	$\gamma = 0.675(10)$	$\gamma = 0.675(8)$
$E_0(\delta) - E_0(\delta = 0)$	$\alpha = 0.95(4)$	$\alpha = 0.97(2)$		